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=> d his full

     (FILE 'HOME' ENTERED AT 15:52:22 ON 11 DEC 2005)

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L1             STRUCTURE UPLOADED
               D QUERY
L2           0 SEA SSS SAM L1 (     0 REACTIONS)
L3           1 SEA SSS FUL L1 (     1 REACTIONS)
               D L3

     FILE 'CAPLUS' ENTERED AT 15:53:15 ON 11 DEC 2005
L4           1 SEA ABB=ON  PLU=ON  L3
               D L4

     FILE 'CASREACT' ENTERED AT 15:53:33 ON 11 DEC 2005
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               D QUERY
L6           0 SEA SSS SAM L5 (     0 REACTIONS)
L7           3 SEA SSS FUL L5 (     3 REACTIONS)
               D L7 1-3

     FILE 'CAPLUS' ENTERED AT 15:55:40 ON 11 DEC 2005
L8           3 SEA ABB=ON  PLU=ON  L7
               D L8 1-3 ABS IBIB


     FILE HOME

     FILE CASREACT
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     26, 1996), unless otherwise indicated in the original publications.

     FILE CONTENT:1840 - 11 Dec 2005 VOL 143 ISS 24

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     FILE CAPLUS

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FILE COVERS 1907 - 11 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 9 Dec 2005 (20051209/ED)

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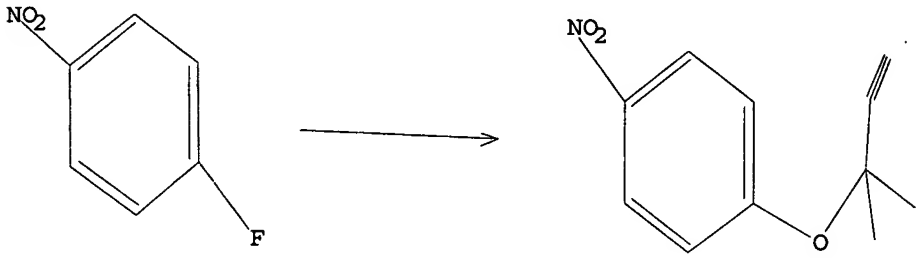

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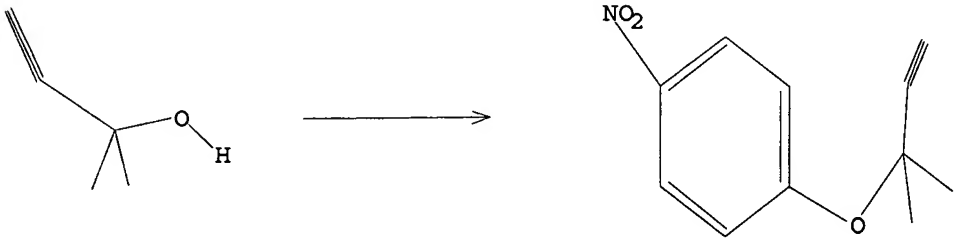
L5 STR



Structure attributes must be viewed using STN Express query preparation.

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

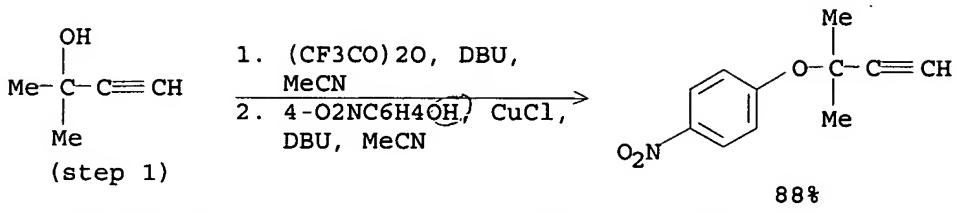
L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

AB An efficient, general, and practical synthesis of aryl 1,1-dimethylpropargyl ethers has been developed. Thus, alkylation of RC6H4OH (R = e.g., 4-CN, 4-NO2) with HC.tplbond.CCMe2X (X = Cl, OCO2Me, O2CCF3) in MeCN containing DBU and Cu salts resulted in high yield of propargyl ethers RC6H4OCMe2C.tplbond.CH (up to 88%).

ACCESSION NUMBER: 1995:65983 CAPLUS
DOCUMENT NUMBER: 122:9577
TITLE: Improved synthesis of aryl 1,1-dimethylpropargyl ethers
AUTHOR(S): Godrey, Jollie D., Jr.; Mueller, Richard H.; Sedergran, Thomas C.; Soundararajan, Nachimuthu; Colandrea, Vincent J.
CORPORATE SOURCE: Chem. Process Research, Bristol-Myers Squibb, Princeton, NJ, 08543-4000, USA
SOURCE: Tetrahedron Letters (1994), 35(35), 6405-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:9577

L7 ANSWER 2 OF 3 CASREACT COPYRIGHT 2005 ACS on STN

RX(4) OF 12



(step 1)

88%

REF: Tetrahedron Letters, 35(35), 6405-8; 1994

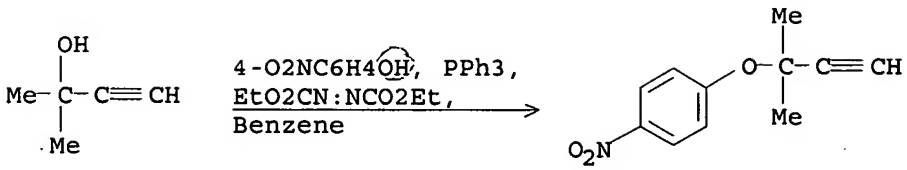
L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

AB The synthesis of aryl ethers of ethynyl carbinols using the Mitsunobu reaction is reported. Thus, a mixture of HC.tplbond.CCMe2OH and 4-MeC6H4OH in C6H6 was treated with Ph3P and EtO2CN:NCO2Et to give 55% 4-MeC6H4OCMe2.tplbond.CH. Eleven similar examples are also reported.

ACCESSION NUMBER: 1990:178193 CAPLUS
DOCUMENT NUMBER: 112:178193
TITLE: A facile synthesis of aryl ethers of ethynyl-carbinols using the Mitsunobu reaction
AUTHOR(S): Subramanian, R. Sankara; Balasubramanian, K. K.
CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Madras, 600 036, India
SOURCE: Synthetic Communications (1989), 19(7-8), 1255-9
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:178193

L7 ANSWER 3 OF 3 CASREACT COPYRIGHT 2005 ACS on STN

RX(7) OF 11



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REF: Synthetic Communications, 19(7-8), 1255-9; 1989

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SESSION RESUMED IN FILE 'REGISTRY' AT 16:34:54 ON 11 DEC 2005
FILE 'REGISTRY' ENTERED AT 16:34:54 ON 11 DEC 2005
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.86	1.07

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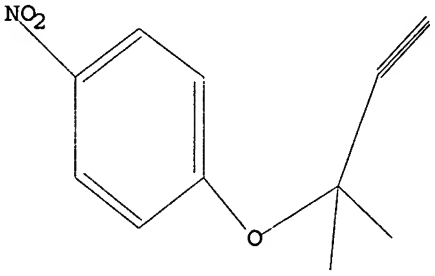
L2 STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

=> s l2 sss full
FULL SEARCH INITIATED 16:36:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> d his

(FILE 'HOME' ENTERED AT 16:32:16 ON 11 DEC 2005)

FILE 'REGISTRY' ENTERED AT 16:32:39 ON 11 DEC 2005
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 0 S L2 SSS SAM
L4 3 S L2 SSS FULL

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	164.34	164.55

FILE 'CAPLUS' ENTERED AT 16:38:28 ON 11 DEC 2005
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FILE COVERS 1907 - 11 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 9 Dec 2005 (20051209/ED)

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=> s l4
L5 9 L4

=> d l5 ibib ab hitstr 1-9

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:1042252 CAPLUS
DOCUMENT NUMBER: 143:326214
TITLE: Preparation of tricyclic benzopyran compounds as anti-arrhythmic agents
INVENTOR(S): Ohrai, Kazuhiko; Shigeta, Yukihiko; Uesugi, Osamu; Okada, Takumi; Matsuda, Tomoyuki
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 445 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090357	A1	20050929	WO 2005-JP6004	20050323

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

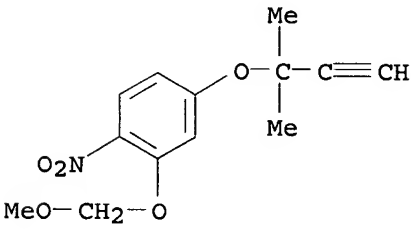
PRIORITY APPLN. INFO.: JP 2004-84605 A 20040323

AB Title compds. I [R1 and R2 independently = H, alkyl or aryl; R3 = H or alkylcarbonyloxy, or together with R4 forms a bond; R4 = H or together with R3 forms a bond, m is an integer of 0 to 4, n is an integer of 0 to 4, V = a single bond, substituted carbon linker, NH, O, etc.; R5 = H or alkyl;, R6 = H, alkyl, cycloalkyl, cycloalkenyl, etc.; R7 and R8 or R8 and R9 together form a 5-, 6- or 7-member unsatd. ring fused with a benzene ring, as the constituent atoms of the ring there may be 1-3 O, N, or S atoms or a combination thereof, with the other R7 or R9 = H], or pharmaceutically acceptable salts thereof, are prepared and disclosed as antiarrhythmic agents. Thus, e.g., II was prepared via dehydrobromination of trans-3-bromo-2,2,7,9-tetramethyl-3,4-dihydro-2H-pyrano[2,3-g]quinolin-4-ol (preparation given) to form the intermediate epoxide which undergoes a regioselective ring opening reaction with 2-phenylethylamine. I selectively prolonged the effective refractory period of the atrium, e.g., II at 0.6 mg/kg prolonged the effective refractory period of the atrium by 21 ms. Pharmaceutical compns. are provided.

IT **865479-08-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tricyclic benzopyran compound as anti-arrhythmic agents)

RN 865479-08-9 CAPLUS

CN Benzene, 4-[(1,1-dimethyl-2-propynyl)oxy]-2-(methoxymethoxy)-1-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:354900 CAPLUS
DOCUMENT NUMBER: 140:357051
TITLE: Process for production of an acetylenic compound
INVENTOR(S): Yamada, Osamu; Matsumoto, Hiroo; Shimizu, Takanori
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035520	A1	20040429	WO 2003-JP12312	20030926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2502360	AA	20040429	CA 2003-2502360	20030926
EP 1564201	A1	20050817	EP 2003-748596	20030926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
NO 2005002392	A	20050718	NO 2005-2392	20050518
PRIORITY APPLN. INFO.:			JP 2002-303876 A	20021018
			WO 2003-JP12312 W	20030926

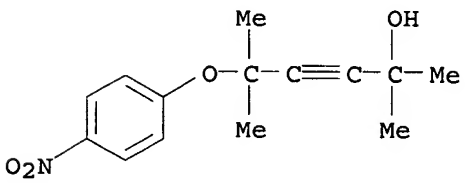
OTHER SOURCE(S): CASREACT 140:357051

AB Disclosed is an industrial and economical process for producing an acetylenic compound (I), namely 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitrobenzene, from 4-nitrofluorobenzene, specifically, characterized by reacting 4-nitrofluorobenzene (II) with an alkoxide of 2-methyl-3-butyn-2-ol (III) at -20 to 10°. The acetylenic compound I is useful as an intermediate for drugs such as an antiarrythmic or antidepressant. Thus, 25.2 g III was added dropwise over 2 h to a suspension of 11.6 g 60% NaH (mineral oil suspension) and 96.0 g N,N-dimethylacetamide with ice-cooling and stirring, and stirred for another 30 min to give a solution of III sodium salt which was treated dropwise with 33.8 g 4-nitrofluorobenzene over 1.5 h under ice-cooling, stirred at the same temperature for 18 h, treated with 480 mL H2O and 480 mL p toluene, shaken to give, after workup and silica gel chromatog., 44.0 g I (90% yield).

IT **682357-24-0P**, 5-(4-Nitrophenoxy)-2,5-dimethyl-3-hexyn-2-ol
RL: BYP (Byproduct); PREP (Preparation)
(process for preparation of 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitrobenzene by etherification of 2-methyl-3-butyn-2-ol metal salt with 4-nitrofluorobenzene)

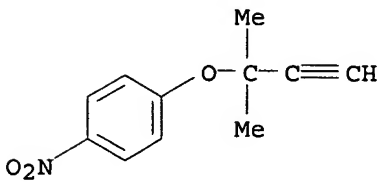
RN 682357-24-0 CAPLUS

CN 3-Hexyn-2-ol, 2,5-dimethyl-5-(4-nitrophenoxy)- (9CI) (CA INDEX NAME)



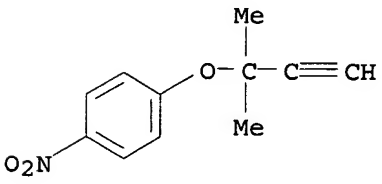
IT **2109-84-4P**, 1-[(1,1-Dimethyl-2-propynyl)oxy]-4-nitrobenzene
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparation of 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitrobenzene by etherification of 2-methyl-3-butyn-2-ol metal salt with 4-nitrofluorobenzene)

RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:650939 CAPLUS
DOCUMENT NUMBER: 123:285380
TITLE: Copper(I) iodide: a catalyst for the improved synthesis of aryl propargyl ethers
AUTHOR(S): Bell, David; Davies, Mark R.; Geen, Graham R.; Mann, Inderjit S.
CORPORATE SOURCE: SmithKline Beecham Pharmaceuticals, Harlow, CM19 5AW, UK
SOURCE: Synthesis (1995), (6), 707-12
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285380
AB Copper(I) iodide catalyzes the reaction between phenols R1C6H4OH (R1 = 4-O2N, 4-I, H, 3-CN, etc.) and dialkylpropargyl chlorides HC.tplbond.CCR2R3Cl [R2 = R3 = Me, Et, CHMe2; R2R3 = (CH2)5; R2 = Me, R3 = Et, CMe3] to give aryl 1,1-dialkylpropargyl ethers, e.g. PhOCMe2C.tplbond.CH, in good yields and purity. These ethers are important as precursors to the 2H-1-benzopyrans.
IT **2109-84-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of aryl propargyl ethers by copper(I) iodide-catalyzed reaction of phenols and dialkylpropargyl chlorides)
RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



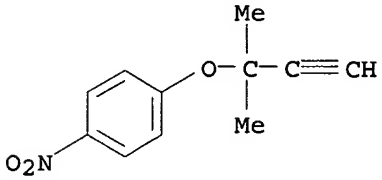
L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:65983 CAPLUS
DOCUMENT NUMBER: 122:9577
TITLE: Improved synthesis of aryl 1,1-dimethylpropargyl ethers
AUTHOR(S): Godrey, Jollie D., Jr.; Mueller, Richard H.; Sedergran, Thomas C.; Soundararajan, Nachimuthu; Colandrea, Vincent J.

CORPORATE SOURCE: Chem. Process Research, Bristol-Myers Squibb, Princeton, NJ, 08543-4000, USA
SOURCE: Tetrahedron Letters (1994), 35(35), 6405-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:9577

AB An efficient, general, and practical synthesis of aryl 1,1-dimethylpropargyl ethers has been developed. Thus, alkylation of RC6H4OH (R = e.g., 4-CN, 4-NO2) with HC.tplbond.CCMe2X (X = Cl, OCO2Me, O2CCF3) in MeCN containing DBU and Cu salts resulted in high yield of propargyl ethers RC6H4OCMe2C.tplbond.CH (up to 88%).

IT **2109-84-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of aryl 1,1-dimethylpropargyl ethers via copper-catalyzed alkylation of phenols with dimethylpropargyl chloride, carbonate, or trifluoroacetate)

RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)

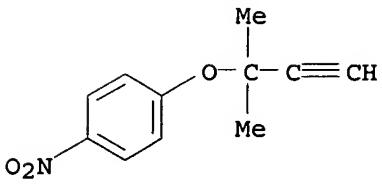


L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:228481 CAPLUS
DOCUMENT NUMBER: 114:228481
TITLE: The synthesis and potassium channel blocking activity of some (4-methanesulfonamidophenoxy)propanolamines as potential class III antiarrhythmic agents
AUTHOR(S): Connors, Sean P.; Dennis, Paul D.; Gill, Edward W.; Terrar, Derek A.
CORPORATE SOURCE: Pharmacol. Dep., Oxford Univ., Oxford, OX1 3QT, UK
SOURCE: Journal of Medicinal Chemistry (1991), 34(5), 1570-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:228481

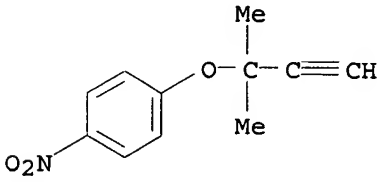
AB The synthesis of 22 (4-methanesulfonamidophenoxy)propanolamines, e.g., I (R = Cl, CF3, etc.) and their testing on isolated guinea pig cardiac myocytes, isolated prepns. from guinea pig atria, and rat blood pressure are described. Secondary amines in the series showed residual β-blocking activity, whereas incorporation of N-Me phenylalkyl and 4-Ph alicyclic amine groups abolished β-blocking activity but led to enhanced ability to block the channel conducting the delayed rectified potassium current, and hence produced an increase in the cardiac action potential duration (APD). Incorporation of hydrophobic Cl and CF3 groups further enhanced potassium channel blocking activity. I (R = Cl, CF3) produced a significant increase in APD at nanomolar concns., with no effect on cardiac muscle conduction velocity, and hence merit further investigation as Class III antiarrhythmic agents. Methylation of the methanesulfonamido group abolished channel-blocking activity; 4-carboxy and 3-methanesulfonamido analogs retained activity but at a reduced level.

IT **2109-84-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:178193 CAPLUS
DOCUMENT NUMBER: 112:178193
TITLE: A facile synthesis of aryl ethers of ethynyl-carbinols using the Mitsunobu reaction
AUTHOR(S): Subramanian, R. Sankara; Balasubramanian, K. K.
CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Madras, 600 036, India
SOURCE: Synthetic Communications (1989), 19(7-8), 1255-9
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:178193
AB The synthesis of aryl ethers of ethynyl carbinols using the Mitsunobu reaction is reported. Thus, a mixture of HC.tplbond.CCMe2OH and 4-MeC6H4OH in C6H6 was treated with Ph3P and EtO2CN:NCO2Et to give 55% 4-MeC6H4OCMe2.tplbond.CH. Eleven similar examples are also reported.
IT **2109-84-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:535107 CAPLUS
DOCUMENT NUMBER: 87:135107
TITLE: Chroman derivatives
INVENTOR(S): Cata, John Morris Evans
PATENT ASSIGNEE(S): Beecham Group Ltd., UK
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2702092	A1	19770728	DE 1977-2702092	19770119

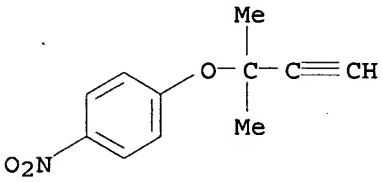
GB 1548221	A	19790704	GB 1976-3024		19761217
FR 2339606	A1	19770826	FR 1977-1699		19770121
FR 2339606	B1	19810116			
AU 7721625	A1	19780803	AU 1977-21625		19770125
DK 7700319	A	19770728	DK 1977-319		19770126
SE 7700824	A	19770728	SE 1977-824		19770126
JP 52091866	A2	19770802	JP 1977-7613		19770126
NL 7700819	A	19770729	NL 1977-819		19770127
PRIORITY APPLN. INFO.:			GB 1976-3024	A	19760127
			GB 1976-14239	A	19760408

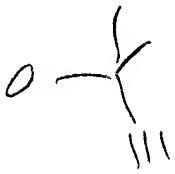
AB Piperidinobenzopyranyl esters I (R = 6-NO2, R1 = Ac, Bz; R = 7-NO2, R1 = Ac) were prepared by esterification. I are antihypertensives. Thus, I (R = 6-NO2, R1 = Bz) at 1 mg/kg orally in rats caused 26% decrease in blood pressure 1 h after administration.

IT **2109-84-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 2109-84-4 CAPLUS

CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



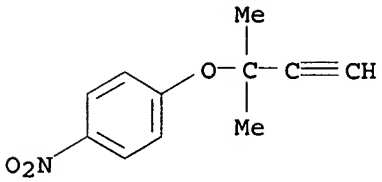


L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1972:126142 CAPLUS
DOCUMENT NUMBER:	76:126142
TITLE:	Influence of structure on the rate of thermal rearrangement of aryl propargyl ethers to the chromenes. Gem-dimethyl effect
AUTHOR(S):	Harfenist, Morton; Thom, Edna
CORPORATE SOURCE:	Burroughs Wellcome Co., Research Triangle Park, NC, USA
SOURCE:	Journal of Organic Chemistry (1972), 37(6), 841-8 CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB The rates of first-order thermal cyclizations of a group of para-substituted aryl propargyl ethers p-ZC6H4OCRR1C.tplbond.CH (R, R1 = H or Me) was determined in 0-Cl2C6H4 as a function of Z (OMe, NHAc, H, Cl, CN, NO2) and of the number of Me groups. Where R and R1 are both H (k values extrapolated to 189.8°) or where R was Me and R1 was H (k values extrapolated to 161.6°), the points followed an adequate Hammett relation using σ+ (ρ = -0.43) although the NO2 and CN did not give a good fit for R = R1 = H, and p-Cl was faster than p-H for R = H, R1 = Me. The attempted Hammett plot for the gem-dimethyl analogs R = R1 = Me had a paraboloid shape, e.g., X = NHAc and X = NO2 had about the same rate, with X = H at a min. (k values extrapolated to 161.6°). The ΔS.++. and ΔH.++. followed no obvious order. The results are best explained by assuming that the gem-dimethyl effect results from an increase in the proportion of the rotamer with the ethynyl group positioned near the benzene ring, i.e., the rotamer best positioned for reaction, when no H is available to rotate to that position, and that activation of the position meta to the substituent Z, at least by the electron-withdrawing groups, exists. Preparative runs showed that an essentially quant. yield of 2-methyl or 2,2-dimethyl-3-chromenes could be obtained.

IT 2109-84-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of cyclization of)
RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)

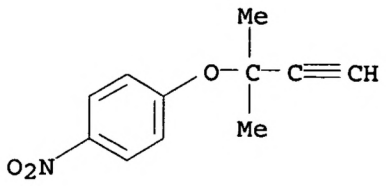


L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:438866 CAPLUS
DOCUMENT NUMBER: 63:38866
ORIGINAL REFERENCE NO.: 63:6917g-h,6918a-b
TITLE: p-tert.-Alkoxyanilines
PATENT ASSIGNEE(S): Wellcome Foundation Ltd.
SOURCE: 20 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6406078		19641201	NL	
PRIORITY APPLN. INFO.:			GB	19630531

AB p-RR1R2COC6H4NR3COR4 (I) is prepared by treating p-O2NC6H4F with KOCRR1R2 to give p-O2NC6H4OCRR1R2 (II), reduction of II to H2NC6H4OCRR1R2 (III), then preparation of p-RR1R2COC6H4NHCOR4 (IV) by adding R4COX to III, and reduction of IV, followed by reaction with R4COX. Thus, 254 g. p-O2NC6H4F was added to 200 g. KOCMe3 in 1200 ml. HOCMe3 and the mixture heated at 100° for 15 min., giving II (R = R1 = R2 = Me) (V), b0.4 112-14°. V(39 g.) in 200 ml. EtOH and 12 g. AcOH was hydrogenated with H (Pt catalyst) to give the corresponding amine, which with 25 g. Ac2O gave IV (R = R1 = R2 = R4 = Me), m. 131-2°. Reduction with Li-AlH4 and reaction with Ac2O gave I (R = R1 = R2 = R4 = Me, R3 = Et), m. 50-3°. Similarly prepared were the following I (R, R1, R2, R3, R4, and m.p. given): Me, Me, Me, H, H, 74°; Me, Me, Me, H, Et, 101°; Me, Me, Me, H, Pr, 126-30°; Me, Me, Me, Me, Me, 80-1°; Me, Me, Me, Pr, Me,- (b0.01 133°); Me, Me, Et, H, Me, 113° (corresponding II b0.03 93-102°); Me, Me, (Me2C(OH)CH2CH2, H, Me, 106-8° (corresponding II b0.2 166-8°); Et, Et, Me, H, Me, 102.6-104° (corresponding II b0.015 98-105°); Me, Me, HC:C, H, Me, 83-4° (corresponding II b0.01 96-100°). These compds. can be used as sedatives and as stimulants.

IT 2109-84-4, Ether, 1,1-dimethyl-2-propynyl p-nitrophenyl
(preparation of)
RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)


Me
O
C
C
CH
Me
O2N